Handout 5 (read by Nov. 20)

Example 2.1.7 In the following we discuss a separation of the Hilbert space of square-integrable functions, $\mathcal{H} = L^2(\mathbb{R}^3)$, using the energy eigenstates of the Hamilton operator corresponding to the three-dimensional harmonic oscillator potential,

$$V(r) = \frac{1}{2} m\omega^2 r^2.$$

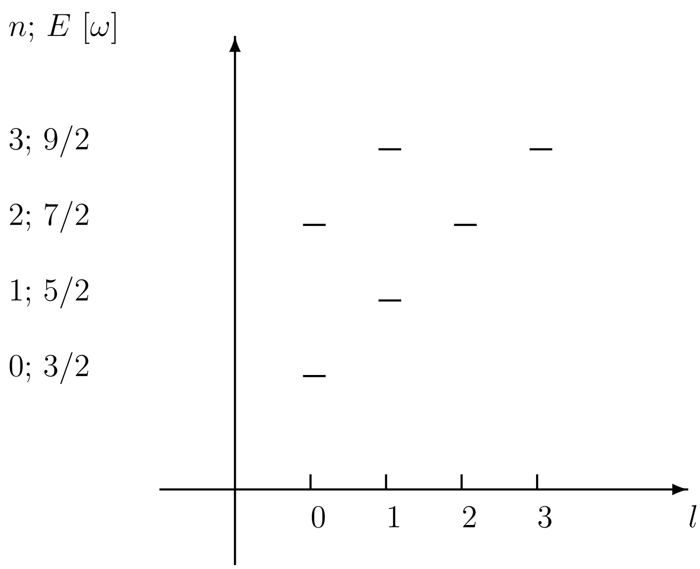

Figure 2.1: Energy eigenvalues E_n of the three-dimensional harmonic oscillator depending on l for $n = 0, \ldots, 3$.

The energy spectrum is given by (see figure 2.1)

$$E_n = \left(n + \frac{3}{2}\right)\omega, \quad n \in \mathbb{N}_0,$$

where $n = 2n_r + l$ denotes the principal quantum number in terms of the radial quantum number n_r and the orbital angular momentum quantum number (or azimuthal quantum number) l.

- The radial quantum number $n_r \geq 0$ corresponds to the number of nodes in the radial wavefunction, where a possible zero at $r = 0$ and the asymptotic zero as $r \to \infty$ are *not* included.
- The orbital angular momentum quantum number l takes values in $\mathbb{N}_0$.

The spectrum of the harmonic oscillator consists entirely of discrete eigenvalues with bound states as the corresponding eigenstates,

$$\psi_{n_r lm}(\vec{x}) = R_{n_r l}(r) Y_{lm}(\theta, \phi) = \langle \vec{x} | n_r, l, m \rangle.$$

For a given l, the radial wave functions are orthogonal,

$$\int_0^\infty drr^2 R_{n_r l}(r) R_{n_r' l}(r) = \delta_{n_r n_r'}. \tag{2.2}$$

In terms of the quantum numbers n_r, l, m the completeness relation reads

$$\mathbb{1} = \sum_{n_r=0}^{\infty} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} |n_r, l, m\rangle\langle n_r, l, m|.$$

Given spherical coordinates,

$$x = r\sin(\theta)\cos(\phi), \quad y = r\sin(\theta)\sin(\phi), \quad z = r\cos(\theta),$$

the angular momentum operators of the position-space representation act exclusively on the angular part of the wave function,

$$\begin{aligned}
\ell_1 &= i\left[\sin(\phi)\frac{\partial}{\partial\theta} + \cot(\theta)\cos(\phi)\frac{\partial}{\partial\phi}\right],\\
\ell_2 &= i\left[-\cos(\phi)\frac{\partial}{\partial\theta} + \cot(\theta)\sin(\phi)\frac{\partial}{\partial\phi}\right],\\
\ell_3 &= -i\frac{\partial}{\partial\phi}.
\end{aligned}$$

The simultaneous eigenfunctions of ℓ_3 and $\vec{\ell}^2$ are given by the spherical harmonics $Y_{lm}(\theta,\phi)$:

$$Y_{lm}(\theta,\phi) := \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}} P_l^m(\cos(\theta)) e^{im\phi}, \tag{2.3a}$$

$$\vec{\ell}^2 Y_{lm}(\theta,\phi) = l(l+1) Y_{lm}(\theta,\phi), \tag{2.3b}$$

$$\ell_3 Y_{lm}(\theta,\phi) = m Y_{lm}(\theta,\phi), \tag{2.3c}$$

where the associated Legendre functions P_l^m are solutions to the general Legendre differential equation. For a given $l \in \mathbb{N}_0$, m takes the values $-l, -l+1, \ldots, l$. Furthermore

$$\ell_\pm Y_{lm}(\theta,\phi) = \sqrt{l(l+1) - m(m\pm1)}\, Y_{l,m\pm1}(\theta,\phi),$$

where

$$\ell_\pm := \ell_1 \pm i\ell_2 = e^{\pm i\phi}\left(\pm\frac{\partial}{\partial\theta} + i\cot(\theta)\frac{\partial}{\partial\phi}\right).$$

The spherical harmonics form an orthonormal and complete set:

$$\underbrace{\int_0^{2\pi} d\phi \int_0^\pi d\theta\, \sin(\theta)}_{=: \int d\Omega} Y^*_{l'm'}(\theta,\phi) Y_{lm}(\theta,\phi) = \delta_{l'l}\delta_{m'm}, \tag{2.4}$$

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y_{lm}^*(\theta',\phi')Y_{lm}(\theta,\phi) = \delta(\phi'-\phi)\delta(\cos(\theta')-\cos(\theta)). \tag{2.5}$$

Let us consider the rotational behavior of a state $|\psi\rangle = |n_r, l, m\rangle$ which is an eigenstate of H, $\vec{\ell}^{\,2}$, and ℓ_3,

$$\begin{aligned}
H|n_r,l,m\rangle &= E_n|n_r,l,m\rangle, \quad n = 2n_r + l,\\
\vec{\ell}^{\,2}|n_r,l,m\rangle &= l(l+1)|n_r,l,m\rangle,\\
\ell_3|n_r,l,m\rangle &= m|n_r,l,m\rangle.
\end{aligned}$$

Using the completeness relation, we express the rotated state as

$$|\psi'\rangle = \mathcal{R}(\alpha,\beta,\gamma)|n_r,l,m\rangle = \sum_{n_r'=0}^{\infty}\sum_{l'=0}^{\infty}\sum_{m'=-l'}^{l'} |n_r',l',m'\rangle\langle n_r',l',m'|\mathcal{R}(\alpha,\beta,\gamma)|n_r,l,m\rangle$$

and consider the matrix element

$$\begin{aligned}
\langle n_r',l',m'|\mathcal{R}(\alpha,\beta,\gamma)|n_r,l,m\rangle &= \int_0^\infty dr r^2 R_{n_r'l'}(r)R_{n_rl}(r)\underbrace{\langle l',m'|\mathcal{R}(\alpha,\beta,\gamma)|l,m\rangle}_{=:\,\delta_{l'l}D^{(l)*}_{m',m}(\alpha,\beta,\gamma)}\\
&= \delta_{l'l}D^{(l)*}_{m',m}(\alpha,\beta,\gamma)\underbrace{\int_0^\infty dr r^2 R_{n_r'l}(r)R_{n_rl}(r)}_{\overset{(2.2)}{=}\,\delta_{n_r'n_r}}\\
&= \delta_{l'l}\delta_{n_r'n_r}D^{(l)*}_{m',m}(\alpha,\beta,\gamma).
\end{aligned}$$

The explanation for the Kronecker delta $\delta_{l'l}$ is as follows:

$$[\vec{\ell}^{\,2},\ell_i] = 0 \;\Rightarrow\; [\vec{\ell}^{\,2}, f(\ell_1,\ell_2,\ell_3)] = 0 \;\Rightarrow\; [\vec{\ell}^{\,2},\mathcal{R}(\alpha,\beta,\gamma)] = 0.$$

Because $\vec{\ell}^{\,2}$ is Hermitian, we can apply it either to the left or to the right,

$$\begin{aligned}
l'(l'+1)\langle l',m'|\mathcal{R}(\alpha,\beta,\gamma)|l,m\rangle &= \langle l',m'|\vec{\ell}^{\,2}\mathcal{R}(\alpha,\beta,\gamma)|l,m\rangle\\
&= \langle l',m'|\mathcal{R}(\alpha,\beta,\gamma)\vec{\ell}^{\,2}|l,m\rangle = l(l+1)\langle l',m'|\mathcal{R}(\alpha,\beta,\gamma)|l,m\rangle.
\end{aligned}$$

We thus obtain

$$\underbrace{[l(l+1)-l'(l'+1)]}_{=(l-l')(l+l'+1)}\langle l',m'|\mathcal{R}(\alpha,\beta,\gamma)|l,m\rangle = 0.$$

From $l + l' + 1 \geq 1$ we conclude for $l \neq l'$:

$$\langle l',m'|\mathcal{R}(\alpha,\beta,\gamma)|l,m\rangle = 0.$$

In other words, we only obtain a contribution for $l = l'$ such that, finally,

$$|\psi'\rangle = \sum_{m'=-l}^{l} D^{(l)*}_{m',m}(\alpha,\beta,\gamma)|n_r,l,m'\rangle,$$

where

$$D^{(l)}_{m,m'}(\alpha,\beta,\gamma) = \langle l,m|\mathcal{R}(\alpha,\beta,\gamma)|l,m'\rangle^*.$$

Remarks

1. The $(2l+1)\times(2l+1)$ matrices $D^{(l)}$ with entries $D^{(l)}_{m,m'}(\alpha,\beta,\gamma)$ form a $(2l+1)$-dimensional representation of the group SO(3). The carrier space is given by the linear span $\mathrm{span}\{|l,m\rangle | m=-l,\ldots,l\}$.

2. In general, for a fixed $l \in \mathbb{N}_0$ a $(2l+1)$-fold degeneracy of energy eigenvalues is a signature of a central potential.

3. The so-called *accidental* degeneracy for $n \geq 2$ is the consequence of a higher symmetry of the system, in the present case an SU(3) symmetry of the three-dimensional harmonic oscillator (see, e.g., Harry J. Lipkin, Lie groups for pedestrians, Dover Publications, Mineola, New York, 2002, chapter 4).

4. The $(2l+1)$-fold degeneracy present for any central potential is referred to as an *essential* degeneracy.

5. The actual energy eigenvalues depend on the dynamics, i.e., the potential.